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EVALUATION OF COMPLEX LOGARITHMS AND RELATED FUNCTIONS. (U)

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AND RELATED FUNCTIONS

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EVALUATION OF COMPLEX LOGARITHMS AND RELATED FUNCTIONS

George J. Miel[†]

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ABSTRACT

An algorithm is presented for computing $\ln z$ with complex arithmetic, by extending to the complex plane Carlson's treatment of a classical iteration using arithmetic and geometric means. Although not competitive with current techniques which handle the real and imaginary parts separately, the algorithm may be useful in special purpose applications. A detailed analysis of convergence, scaling, and roundoff is given. Standard identities and some minor bookkeeping allow the evaluation of inverse circular and inverse hyperbolic functions. It is also shown that the basic procedure is related to certain real algorithms.

AMS (MOS) Subject Classifications: 65D20, 30-04, 65B05

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SIGNIFICANCE AND EXPLANATION

Complex logarithms are usually computed with real arithmetic,

$$\ln(x + iy) = \frac{1}{2} \ln(x^2 + y^2) + i \tan^{-1}(y/x) ,$$

using the real \ln and real \tan^{-1} functions available in high level programming languages. This report studies a novel approach, based on complex arithmetic, obtained by extending to the complex plane a known real algorithm. The strategy consists of a basic iteration, which uses one complex square root per cycle, accelerated by Richardson extrapolation, a speeding-up process well-known to numerical analysts. With proper scaling of the argument, the accelerated procedure requires four complex square roots for accuracy to 10 decimals (compared to eighteen complex square roots in the non-accelerated case). Standard identities such as

$$\cosh^{-1} z = \ln(z + \sqrt{z^2 - 1}) ,$$

$$\cos^{-1} z = i \cosh^{-1} z ,$$

etc.

and some minor bookkeeping to account for principal branches, allow the evaluation of complex inverse trigonometric functions. The report analyzes the algorithm with respect to scaling, convergence, and stability, and it relates the algorithm to other procedures, including classical methods for calculating the constant π . Since complex square roots are done at the software level, and thus costly in machine time, the algorithm is not competitive with standard methods handling the real and imaginary parts separately with real arithmetic. However, its simplicity and stability could make it attractive for implementation in microcode or read only memory in special purpose applications requiring extensive use of elementary complex functions.

The responsibility for the wording and views expressed in this descriptive summary lies with MSA, and not with the author of this report.

EVALUATION OF COMPLEX LOGARITHMS AND RELATED FUNCTIONS

George J. Miel[†]

1. Introduction. Logarithms of complex numbers are commonly computed using real arithmetic separately for the real and imaginary parts,

$$\ln(x + iy) = \frac{1}{2} \ln(x^2 + y^2) + i \tan^{-1}(y/x) , \quad (1.1)$$

with suitable precautions to avoid numerical problems; see, e.g., [6, Algorithm 243]. We analyze an algorithm based on complex arithmetic, obtained by extending to the complex case Carlson's procedure [3]. The strategy consists of a basic iteration, which uses one complex square root per cycle, accelerated by Richardson extrapolation. The basic iteration generates one of the sequences of Borchardt's algorithm [2, p. 499], [4, p. 170]. For real arguments, this iteration is also related to Thacher's algorithm for inverse cosines [11], to Viète's infinite product for π [8, p. 26], and to the method of equal perimeters [8, p. 32]. As for the real case, the improvement due to extrapolation is substantial, the algorithm is reliable and stable, and storage needs are modest as there are no constants to be saved. Numerical experiments indicate no serious cancellation leading to loss of significant figures, as sometimes happens when a real algorithm is extended to the complex case. With an adequate reduction in the range of the independent variable, the accelerated procedure requires four complex square roots for 10D accuracy. Standard identities, and some bookkeeping to account for principal branches, allow the evaluation of inverse circular and inverse hyperbolic functions. The complex arithmetic

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provides a unified design for a simple and modular software package. Unfortunately, the complex square roots preclude the algorithm from competition with the straightforward approach (1.1), which takes advantage of efficient real elementary functions provided in high level languages. However, the algorithm might be of interest in special purpose applications implemented in microcode or read only memory. Certain monotonicity properties of Borchardt's iteration can be exploited for computation in complex interval arithmetic [10].

2. The Basic Algorithm. The goal is to evaluate the single-valued function $\ln z$ whose range is $\{x + iy \mid -\pi \leq y < \pi\}$. The rational operations of complex arithmetic and the principal complex square root are assumed available [6, Key A2]. The latter is the single-valued function whose range is

$$\mathbb{C}^+ = \{x + iy \mid x > 0 \text{ or } x=0 \text{ with } y \geq 0\}.$$

Recall that

$$\sqrt{z^2} = z, \text{ if } z \in \mathbb{C}^+. \quad (2.1)$$

We will use the function $F(z) = (z \coth z)/w$ and its expansion

$$F(z) = a_0 + a_1 z^2 + a_2 z^4 + \dots + a_m z^{2m} + o(z^{2m+2}), \quad (2.2)$$

where a_j depends on the Bernoulli number B_{2j} ,

$$a_j = \frac{2^{2j} B_{2j}}{(2j)! w},$$

and where Landau's notation $f(z) = o(g(z))$ is adequately defined [7, p. 156].

In what follows, $D = \{z \mid |z| > 1\}$.

Theorem. Let $z \in D$ and

$$\xi_0 = \frac{z+1}{z-1}, \quad \xi_{n+1} = \xi_n + \sqrt{\xi_n^2 - 1}, \quad n \geq 0. \quad (2.3)$$

The numbers ξ_n satisfy

$$\xi_n = \coth 2^{-n-1} w, \quad \xi_{n+1} = 2\xi_n + \epsilon_n, \quad (2.4)$$

where $w = \ln z$, $\epsilon_n = -1/\xi_{n+1}$, $|\epsilon_n| \ll |\xi_n|$, and the numbers $u_n = 2^{-n-1} \xi_n$

converge to $u = 1/w$ with a rate

$$u - u_{n+1} = 4^{-n-1} (u - u_n) + o(16^{-n-1}). \quad (2.5)$$

Proof. For $n = 0$, $\xi_0 = (e^w + 1)/(e^w - 1) = \coth w/2$. The relation $\zeta = a + ib$, $\operatorname{csch} \zeta = |\sinh \zeta|^{-2} (\sinh a \cos b - i \cosh a \sin b)$ implies that $\operatorname{csch} w/2 \in \mathbb{C}^+$ whenever $w \in \ln(D)$. Use the identities $\coth \zeta/2 = \coth \zeta + \operatorname{csch} \zeta$, $\operatorname{csch}^2 \zeta = \coth^2 \zeta - 1$ and (2.1) to get

$$\coth w/4 = \coth w/2 + \sqrt{\coth^2 w/2 - 1}, \quad w \in \ln(D).$$

The relation (2.3) gives $\xi_{n+1} = 2\xi_n - 1/\xi_{n+1}$. The convergence follows from $u_n = F(2^{-n-1}w)$ and $\lim_{\zeta \rightarrow 0} F(\zeta) = 1/w$. Finally, use (2.2) with $m = 1$ to get (2.5).

The second expression in (2.4) shows that as n increases, ξ_{n+1} gets increasingly close to $2\xi_n$. This fact provides a simple variable precision scheme. A range reduction allows the evaluation of logarithms for machine representable arguments.

Basic Algorithm. Adequate precision is assumed available. Given $z' \neq 0$, proceed as follows to find $\ln z'$ correct to d decimals:

1. Factorize $|z'| = 2^r x$, $x \in [2, 4)$. Let $z = 2^{-r} z'$.
2. Compute (2.3) with $n = 0, 1, \dots, N$ where N is such that ξ_N and $2\xi_{N-1}$ agree to $d + 1$ decimals.
3. Let $\ln z' = (2^{-N-1}\xi_N)^{-1} + r \ln 2$.

Various range reductions are possible. Instead of the modulus, one can use $|a + ib| = |a| + |b|$ or $|a + ib| = \max(|a|, |b|)$. The code should take advantage of the multiplications by powers of 2.

Roundoff Propagation. Numerical experiments indicate that the algorithm is remarkably stable. A simplified analysis shows why. Consider

$$\hat{\xi}_0 = \xi_0 - \varepsilon_0, \quad \hat{\xi}_{n+1} = \phi(\hat{\xi}_n) - \delta_n, \quad \hat{u}_n = 2^{-n-1}\hat{\xi}_n,$$

where $\phi(z) = z + \sqrt{z^2 - 1}$ and δ_n reflects the accuracy of the complex square root routine. Letting $\epsilon_n = \xi_n - \hat{\xi}_n$,

$$\epsilon_{n+1} \approx \phi'(\xi_n)\epsilon_n + \delta_n, \quad \phi'(\xi_n) = \xi_{n+1}/(\xi_{n+1} - \xi_n).$$

Since $\xi_{n+1} \approx 2\xi_n$, assume for simplicity that $\delta_n \approx 2\delta_{n-1}$, $\phi'(\xi_n) \approx 2$.

Then $\epsilon_N \approx N2^{N-1}\delta_0 + 2^N\epsilon_0$, and assuming no error in the multiplication by 2^{N-1} , we get

$$u_N - \hat{u}_N \approx \frac{N}{4}\delta_0 + \frac{\epsilon_0}{2}. \quad (2.6)$$

The accumulated roundoff is acceptable if the square root routine is accurate to at least $d + 2$ decimals. Practice shows that cancellation causes actual roundoff to be smaller than (2.6).

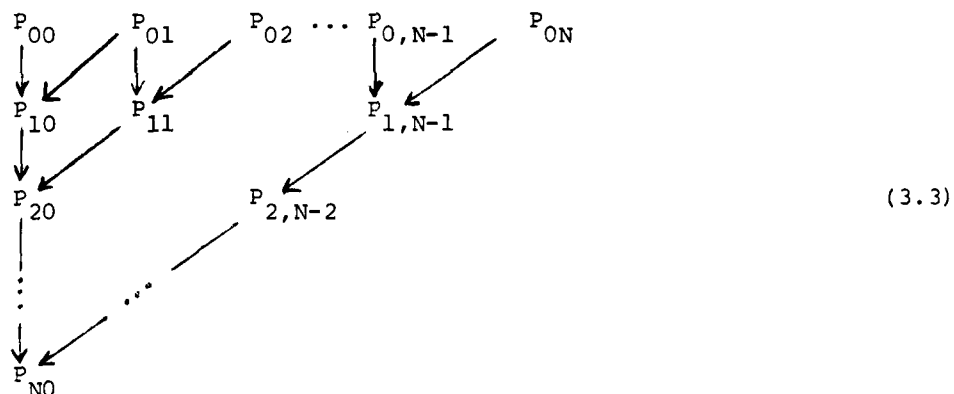
3. Richardson Extrapolation. Section 5 shows that $\{u_n\}$ is one of the sequences generated by Borchardt's algorithm [2], [3], [4, p. 170]. As for the real case, (2.5) indicates that successive errors in u_n are ultimately reduced by a factor 1/4. In order to speed-up convergence, we extend to the complex case the treatment of Carlson [3].

The procedure is given by

$$P_{0n} = u_n, \quad 0 \leq n \leq N, \quad (3.1)$$

$$P_{kn} = P_{k-1,n+1} + \frac{P_{k-1,n+1} - P_{k-1,n}}{4^k - 1}, \quad \begin{matrix} 1 \leq k \leq N \\ 0 \leq n \leq N-k \end{matrix} \quad (3.2)$$

The scheme generates a triangular array,



in which the arrows illustrate the dependence of P_{kn} on $P_{k-1,n}$ and $P_{k-1,n+1}$.

Recall that for $z \in D$, $u_n = F(\zeta_n) \rightarrow u = 1/w$, $\zeta_n = w/2^{n+1}$.

Let

$$F_0(\zeta) = F(\zeta), \quad F_k(\zeta) = \frac{4^k F_{k-1}(\zeta) - F_{k-1}(2\zeta)}{4^k - 1}.$$

Then (2.2) implies that

$$F_k(\zeta) = u + b_k \zeta^{2k+2} + O(\zeta^{2k+4}),$$

where b_k is a constant. Since $\zeta_n = 2 \zeta_{n+1}$, we have $P_{kn} = F_k(\zeta_{n+k})$. Consequently,

$$P_{kn} - u = 4^{-(k+1)(k+n+1)} b_k w^{2k+2} + O(4^{-(k+2)(k+n+1)}).$$

Thus, the errors in successive elements of the k -th row of (3.3) are each time roughly reduced by a factor $4^{-(k+1)}$.

Error Bounds via Interpolation Theory. Let $f(z) = F(\sqrt{z}) = (\sqrt{z} \coth \sqrt{z})/w$ and $z_n = \zeta_n^2 = w^2/4^{n+1}$; (3.2) is the Neville scheme for evaluating polynomials with

P_{kn} = value at $z=0$ of the polynomial of degree $\leq k$

which interpolates $f(z)$ at $z_n, z_{n+1}, \dots, z_{n+k}$;

see Brezinski [1, p.26]. The function $f(z)$ is analytic for $|z| < \pi^2$.

Theorem. If $u = 1/w$, $w = \ln z$, and

$$1 < |z| \leq e^{\sqrt{7\pi^2 - 18}/3} \quad (3.4)$$

then

$$|u - P_{kn}| < 2^{-(k+1)(k+2n+1)} |w|^{2k+1} \left(\frac{|w|^2}{2} + \pi \right). \quad (3.5)$$

Proof. Let $a = \frac{2\pi}{3}$ and let C'' denote the square with vertices $a(\pm 1 \pm i)$. We first show that

$$\max_{z \in C''} |\coth z| \leq \coth a. \quad (3.6)$$

For the side $z = a + iy$, $-a \leq y \leq a$, we get

$$|\coth z| \leq \frac{|e^{a+iy}| + |e^{-a-iy}|}{||e^{a+iy}| - |e^{-a-iy}||} = \frac{e^a + e^{-a}}{e^a - e^{-a}} = \coth a.$$

For $z = x + ia$, $-a \leq x \leq a$, use $e^{ia} = \frac{1}{2}(-1 + i\sqrt{3})$ to obtain

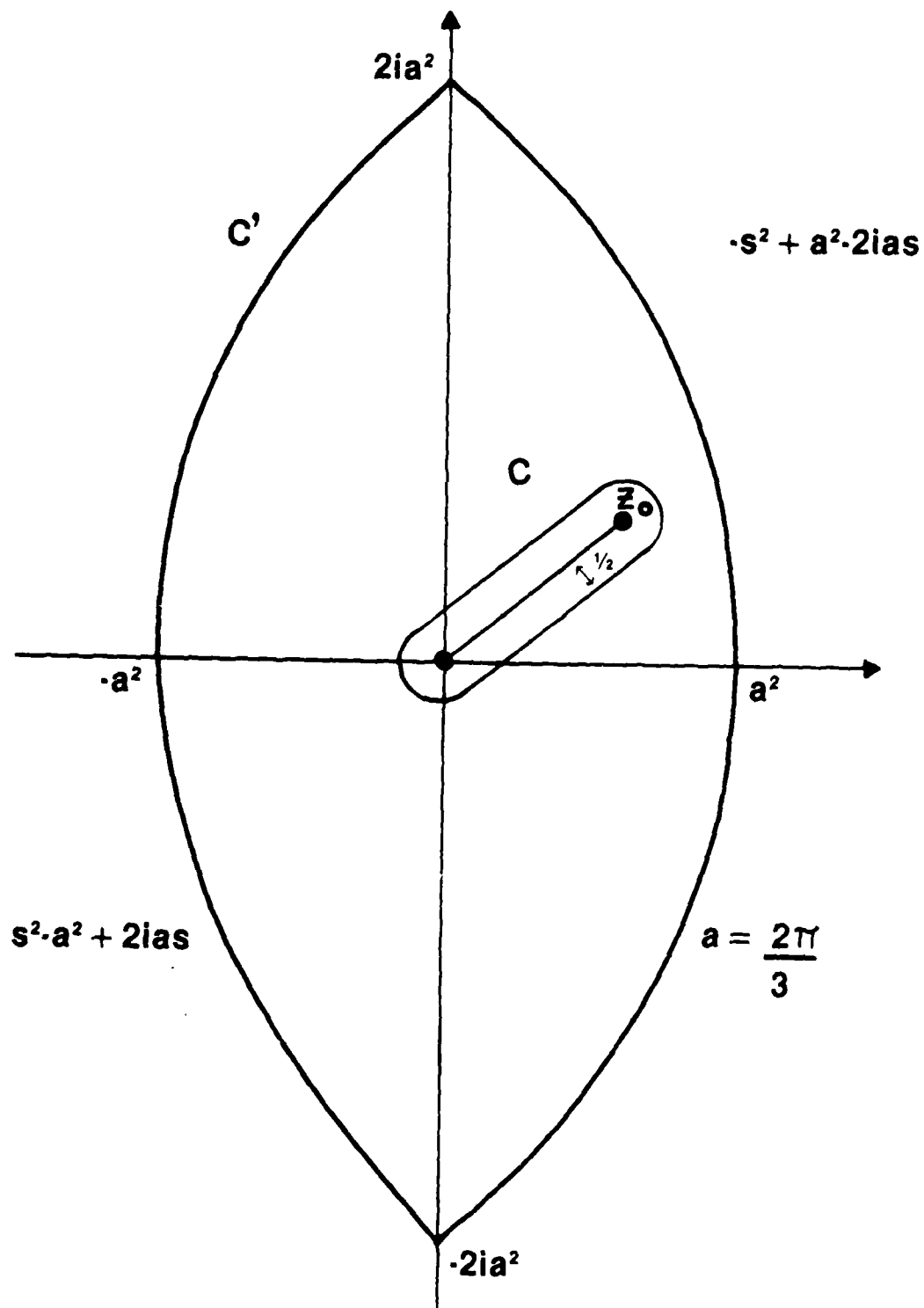


FIG. Estimate $\max |\sqrt{t} \coth \sqrt{t}|$ for $t \in C'$ rather than $t \in C$ using that \sqrt{t} is then on the square C'' .

$$|\coth z| = \left| \frac{1 - i\sqrt{3} \tanh x}{\tanh x - i\sqrt{3}} \right| = \left(\frac{3 \tanh x + 1}{\tanh^2 x + 3} \right)^{1/2} \equiv \psi(x).$$

Similarly for the other two sides. The function $\psi(x)$ reaches its maximum at $x=ia$. Since $\psi(ia) < \coth a$, we get (3.6).

Now, let C denote the union of two semicircles of radius $1/2$ and centers at 0 and $z_0 = \frac{w^2}{4}$ respectively, and two parallel segments as shown in the figure. Consider also the union of two partial parabolas,

$$C' = \{ \pm(s^2 - a^2 + 2ias) \mid -a \leq s \leq a \}.$$

The curve C' is inside the circle of analyticity and (3.4) implies that C is not outside C' .

By a classic result,

$$u - p_{kn} = \frac{(-1)^{k+1}}{2\pi i} \cdot \frac{z_n z_{n+1} \cdots z_{n+k}}{w} \cdot I, \quad (3.7)$$

where

$$I = \int_C \frac{g(t) dt}{t(t-z_n) \cdots (t-z_{n+k})}, \quad g(t) = \sqrt{t} \coth \sqrt{t}.$$

But

$$|I| \leq 2^{k+2} (2|z_0| + \pi) M, \quad (3.8)$$

where $M \geq \max_{t \in C} |g(t)|$. We have

$$\max_{t \in C} |g(t)| \leq \max_{t \in C} |g(t)| = \max_{z \in C} |g(z^2)| \leq \sqrt{2} a \coth a \approx 0.972 \pi,$$

where we used (3.6). To complete the proof, take $M = \pi$ and use (3.7) and (3.8).

For the range reduction described earlier, (3.4) is satisfied and

$|w| < |\ln 4 + i\pi|$. For accuracy to d decimals, set the bound in (3.5) no greater than $\frac{1}{2}10^{-d}$ and thus obtain:

Non-accelerated case ($k=0, n=N$) $N \geq 1.66 d + 2.48,$

Accelerated case ($k=n=N$) $N \geq \sqrt{1.11 d + 1.66} - 0.07.$

Actual computation shows that 10D accuracy requires $N = 18$ in the non-accelerated case and $N = 4$ in the extrapolated case. The acceleration defined by (3.1) and (3.2) is easily coded. The code should take advantage of the multiplications by powers of 4. Variable precision is possible by a priori specification of N or by on-line comparison of P_{NO} and $P_{N-1,1}$.

Roundoff Propagation. If the values in the first row of (3.3) are contaminated with errors whose magnitudes are less than ϵ , then the errors later in the extrapolation have magnitude which nowhere exceed 2ϵ . Combining this with (2.6), we get

$$|P_{NO} - \hat{P}_{NO}| \lesssim \left| \frac{N}{2} \delta_0 + \epsilon_0 \right| + |\zeta|,$$

where \hat{P}_{NO} is the computed value of P_{NO} and ζ is the accumulated roundoff in the computation of (3.2). The major term is $\frac{N}{2} \delta_0$ and the extrapolation is well-conditioned provided that the square root routine is of good quality.

4. Inverse Trigonometric Functions. The table below specifies for each function a bijection between the domain and given range.

| FUNCTION | RANGE |
|--------------|---|
| \ln | $R_1 = \{a+ib \mid -\pi \leq b < \pi\}$ |
| \cosh^{-1} | $R_2 = \{a+ib \mid -\pi < b < 0 \text{ or } b = -\pi, 0 \text{ with } a \geq 0\}$ |
| \sinh^{-1} | $R_3 = \{a+ib \mid -\pi/2 < b < \pi/2 \text{ or } b = \pm \pi/2 \text{ with } a \geq 0\}$ |
| \tanh^{-1} | $R_4 = \frac{1}{2} R_1 - \{-i\pi/2\}$ |
| \cos^{-1} | iR_2 |
| \sin^{-1} | iR_3 |
| \tan^{-1} | $-iR_4$ |

The following procedures use standard identities to evaluate the functions.

Algorithm for $w = \cosh^{-1} z$.

$$w' = \ln(z + \sqrt{z^2 - 1}) = a + ib.$$

If $b > 0$ then $w = -w'$.

If $b = -\pi, 0$ and $a < 0$ then $w = -a + ib$.

Otherwise, $w = w'$.

Algorithm for $w = \cos^{-1} z$.

$$w = i \cosh^{-1} z.$$

Algorithm for $w = \tanh^{-1} z$.

$$z \neq \pm 1, w = \frac{1}{2} \ln\left(\frac{1+z}{1-z}\right).$$

Algorithm for $w = \sinh^{-1} z$.

$$w' = \ln(z + \sqrt{z^2 + 1}) = a + ib.$$

If $b \in [-\pi, -\pi/2)$ then $w = -i\pi - w'$.

If $b \in (\pi/2, \pi)$ then $w = i\pi - w'$.

If $b = \pm\pi/2$ and $a < 0$ then $w = -a + ib$.

Otherwise, $w = w'$.

Algorithm for $w = \sin^{-1} z$.

$$w = i \sinh^{-1}(-iz).$$

Algorithm for $w = \tan^{-1} z$.

$$z \neq \pm i, w = -i \tanh^{-1} iz.$$

In the case of \cosh^{-1} and \sinh^{-1} , some logic is needed in order to choose the value in the specified range, since these functions are double-valued in the range of \ln , [9, p. 417].

5. Connection with Real Algorithms. For real arguments, our accelerated procedure is exactly equivalent to Carlson's treatment of Borchardt's algorithm [3]. The non-accelerated procedure is related to Thacher's algorithm [11] for real inverse cosines and to classical methods for calculating π .

Borchardt's Algorithm. If $u_{-1}, v_{-1} > 0$ then the sequences

$$u_{n+1} = \frac{1}{2}(u_n + v_n), \quad v_{n+1} = \sqrt{u_{n+1} v_n}, \quad n \geq -1, \quad (5.1)$$

converge monotonically to a common limit $B(u_{-1}, v_{-1})$, [2]. We show that

$$u_n = 2^{-n-1} \xi_n, \quad \xi_{n+1} = \xi_n + \sqrt{\xi_n^2 - u_{-1}^2 + v_{-1}^2}. \quad (5.2)$$

Get the invariant $4^{n+1}(u_{n+1}^2 - v_{n+1}^2) = c$ and then substitute $v_n = (u_n^2 - 4^{-n}c)^{1/2}$

in the first relation of (5.1). Our basic algorithm generates (5.2) corresponding to

$$B\left(\frac{z^2+1}{z^2-1}, \frac{2z}{z^2-1}\right) = \frac{1}{\ln z}.$$

Thacher's Algorithm. If $R_1 = \sqrt{2z+2}$, $R_{n+1} = \sqrt{R_n+2}$ then $t_n = 2^n \sqrt{R_n-2}$

converge to $\cos^{-1} z$ if $|z| < 1$ and to $\cosh^{-1} z$ if $|z| \geq 1$, [11]. It turns

out that t_n is the reciprocal of v_n generated by (5.1) with proper u_{-1} and v_{-1} .

Method of Equal Perimeters. If $\mu > 2$ then

$$B\left(\frac{1}{\mu} \cot \frac{\pi}{\mu}, \frac{1}{\mu} \csc \frac{\pi}{\mu}\right) = \frac{1}{\pi},$$

$$u_n = \frac{1}{2^{n+1}\mu} \cot \frac{\pi}{2^{n+1}\mu} = \text{radius of inscribed circle in a regular } 2^{n+1}\mu\text{-gon of perimeter 2.}$$

Descartes worked with $\mu = 4$, [8, p.32].

Viète's Infinite Product. If $g_{-1} = \sqrt{2}$, $g_0 = \sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{\frac{1}{2}}}$, $g_n = \sqrt{\frac{1}{2} + \frac{1}{2}g_{n-1}}$

then $\lim(g_{-1}g_0 \dots g_n) = 4/\pi$, [8, p.26]. We have $g_{-1}g_0 \dots g_n = v_n$, where v_n

corresponds to $B(1, \sqrt{2}) = 1/\sin^{-1}\sqrt{\frac{1}{2}}$.

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